A Game of Order Parameters - Crystal Nucleation

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Motivation

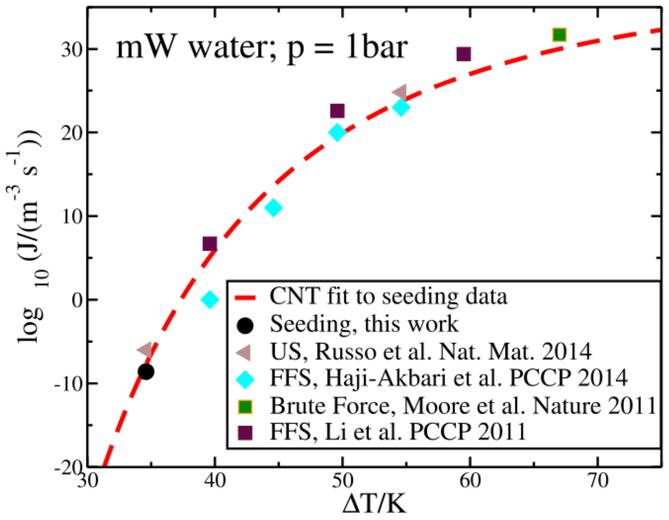

Figure 1: Espinosa *et al* JCP, **2016**, 144, 034501. Nucleation rates of mW water, obtained from various studies

- Current nucleation data differs by orders of magnitude, with little/no uncertainty quantification
- Unclear if choice of order parameter (mathematical object defining crystalline cluster) impacts on this

Initial Workplan

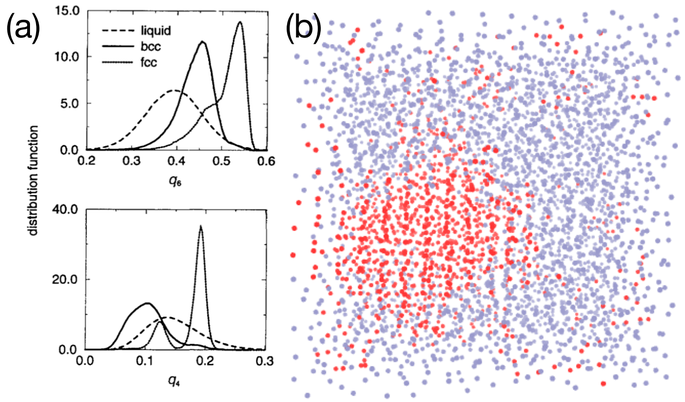

Figure 2: (a) Ten Wolde *et al* Faraday Discuss., **1996**, 104, 93. Distribution functions for two different order parameters, P(q_6) and P(q_4). *(b)* Snapshot of solid atoms (red) growing inside a liquid (blue)

- Start with a Lennard-Jones system, and investigate the effect of different order parameters

Current Work

- Forward flux sampling (FFS) initial flux

  ➡ Count how many times nucleus grows to exceed λ_0 atoms

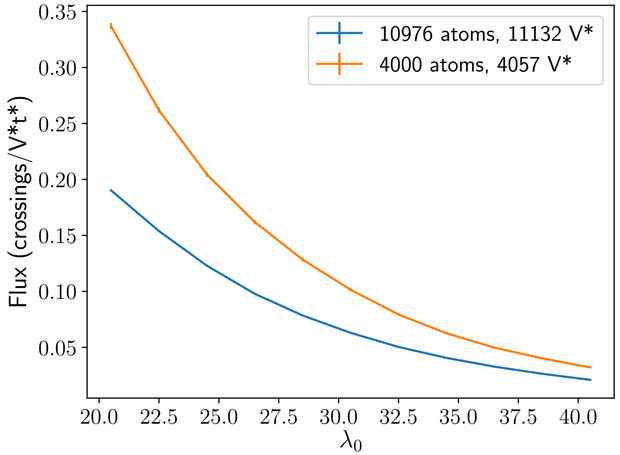

Figure 3: Comparison of initial flux of Lennard-Jones systems at two different volumes as a function of the cluster size of the interface (λ_0)

- Previously unknown size dependence of flux through initial interface.